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Boundary Value Methods: The Third Way Between Linear Multistep and Runge-Kutta Methods

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Abstract—It is well known that the approximation of the solutions of ODEs by means of k-step methods transforms a first-order continuous problem in a k^{th}-order discrete one. Such transformation has the undesired effect of introducing spurious, or parasitic, solutions to be kept under control. It is such control which is responsible of the main drawbacks (e.g., the two Dahlquist barriers) of the classical LMF with respect to Runge-Kutta methods. It is, however, less known that the control of the parasitic solutions is much easier if the problem is transformed into an almost equivalent boundary value problem. Starting from such an idea, a new class of multistep methods, called Boundary Value Methods (BVMs), has been proposed and analyzed in the last few years. Of course, they are free of barriers. Moreover, a block version of such methods presents some similarity with Runge-Kutta schemes, although still maintaining the advantages of being linear methods. In this paper, the recent results on the subject are reviewed. © 1998 Elsevier Science Ltd. All rights reserved.

Keywords—Numerical methods for ODEs, Linear multistep formulae, Boundary value methods, Discrete boundary value problems.

1. INTRODUCTION

It is well known that Runge-Kutta (RK) methods are more flexible than Linear Multistep Formulae (LMF) as traditionally used. Among the drawbacks suffered by LMF, we recall the following ones:

(1) the Dahlquist barriers,
(2) the impossibility to define stable, high-order symplectic methods,
(3) difficulties when changing the stepsize.

On the contrary, they have some advantages over the rival class, such as the easier analysis of their properties and the same accuracy at each point (they have no internal point to discard).

In recent years, LMF have been generalized as described below. The resulting methods, called boundary value methods (BVMs), no longer suffer the limitations described at points 1 and 2. Furthermore, their block implementation permits us to avoid the third difficulty as well. Consequently, we have A-stable, essentially symplectic BVMs of any order.

In this paper, we shall review some recent results in this field. In Section 2, we shall describe the underlying idea on which BVMs are based, along with the generalizations to the new setting of the classical results about stability and convergence. In Sections 3 and 4, two of the most popular families of LMF, that is, the backward differentiation formulae and Adams-Moulton methods, are generalized in order to take the maximum advantage from the new formulation. In Section 5, we examine symmetric schemes, which provide methods well suited for approximating

Hamiltonian problems. In Section 6, the problem of the choice of the additional conditions will be briefly examined. In Section 7, the block version of the methods is introduced. Finally, in Section 8, some numerical results are presented.

2. BOUNDARY VALUE METHODS

The main concern of Numerical Analysis is to detect ill-conditioned problems and avoid them, whenever possible. Ill-conditioned problems are those for which there exists a relation between a measure of the solution and a measure of the data, but a small perturbation on the latter causes a large perturbation on the former. To fix the idea, let us consider the simple problem

$$y'' = 9y' + 10y, \qquad y(0) = \frac{1}{3}, \qquad y'(0) = -\frac{1}{3}, \tag{1}$$

whose solution is $y(t, 0, 1/3, -1/3) = e^{-t}/3$. In this case, a small perturbation on the data will cause a large perturbation on the solution. For example, to a perturbation of a small amount ε of the first initial condition, it corresponds the solution

$$y\left(t, 0, \frac{1}{3} + \varepsilon, -\frac{1}{3}\right) = \left(\frac{1}{3} + \frac{10}{11}\varepsilon\right) e^{-t} + \frac{\varepsilon}{11} e^{10t}.$$

In Figure 1, the geometry around the solution is shown. Such a situation is dangerous if one needs to obtain some quantitative result, other then a qualitative information. For example, the use of finite precision arithmetic will introduce errors and, then, the computed solution will be far from the desired one.

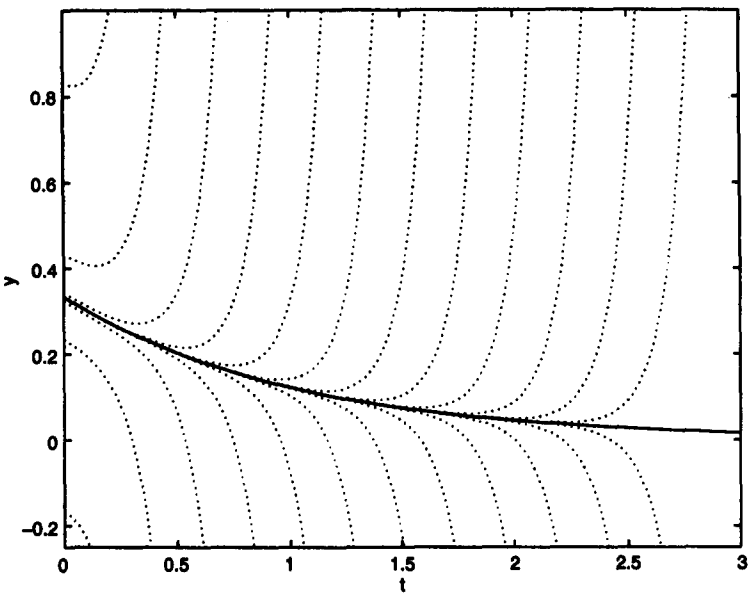

Figure 1. Geometry around the solution of problem (1).

Is there a possibility to improve the geometry around the solution? Yes, if we are willing to pay a little. In fact, there are boundary value problems whose solutions are as near as we like to $e^{-t}/3$, but having much better geometries around it. That is, they are much better conditioned. Let us consider, for example, the same equation with the following boundary conditions:

$$y(0) = \frac{1}{3}, \qquad y(T) = 0. \tag{2}$$

The solution now is

$$y(t) = \frac{1}{3}\frac{e^{-t}}{1 - e^{-11T}} - \frac{e^{-T}}{3}\frac{e^{10(t-T)}}{1 - e^{-11T}} \approx \frac{1}{3}e^{-t}, \qquad \text{for } t \ll T.$$

As a consequence, for T enough larger than the interval of interest, such solution will differ from the solution $e^{-t}/3$ less than any prefixed tolerance. Despite the fact, that now the solution only approximates the function $e^{-t}/3$, the problem is much better conditioned. The difference is that now the surrounding geometry is much smoother, as shown in Figure 2. As a consequence, any quantitative evaluation will be much safer.

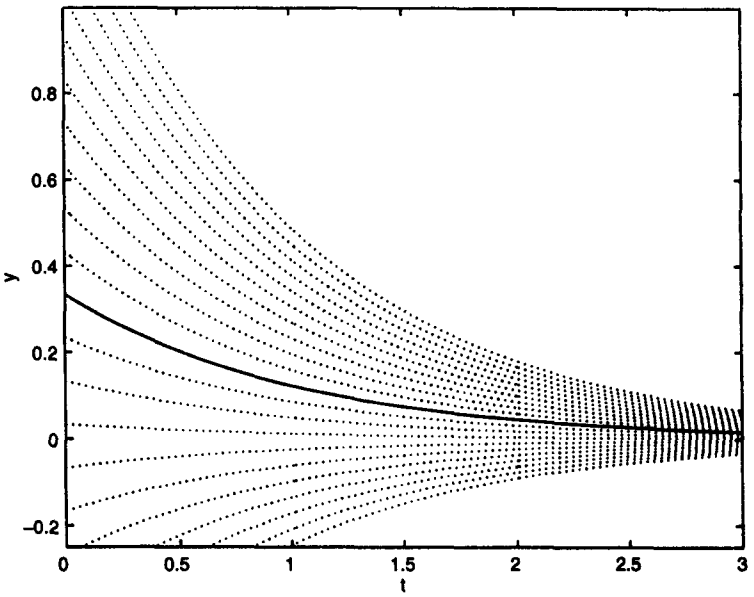

Figure 2. Geometry around the solution by using the boundary conditions (2), $T = 5$.

The reason of the different geometry around the solution relies on the fact that the considered boundary value problem selects, in the space of solutions, only those having a decaying behavior, as the one in which we are interested. However, the idea works, as it can be easily proved, also in the case where the space of solutions contains only decaying (or only increasing) solutions with different time scales.

The above discussion may be generalized to the case where more than two different modes are present, that is the case of higher-order differential equations. In other words, appropriate boundary value problems permit to select in a safe way (i.e., by means of well-conditioned problems) particular solutions of intermediate grow rate.

The same happens for discrete problems. That is, appropriate discrete boundary value problems can be used to approximate particular solutions better than initial value problems.

This idea was used in the fifties by Miller [1] to get the numerical evaluation of Bessel functions, which, as it is well known, satisfy second-order difference equations.

It is then not surprising, the use of multistep methods with boundary conditions to approximate continuous initial value problems.

As matter of fact, when a well-conditioned first-order continuous problem

$$y' = f(t, y), \qquad y(t_0) = y_0 \tag{3}$$

is approximated by a difference equation of higher order, as it is the case of multistep methods, parasitic modes are introduced in the discrete problem. The main concern will be to get rid of them. It is the control of such parasitic modes which is responsible of the Dahlquist barriers.

In fact, when the method is applied to the usual scalar test equation

$$y' = \lambda y, \tag{4}$$

where $\mathrm{Re}(\lambda) < 0$, and the resulting difference equation is used as initial value problem, such control requires all the roots of the characteristic polynomial to be inside the unit circle of the

complex plane. This is a severe restriction since it conflicts with the precision (order) conditions. On the contrary, the use of a boundary value problem allows some of the roots to lie outside the unit disk. Such freedom makes less conflicting the stability and the order conditions.

Consider, for example, the simple initial value problem (4) with $\lambda < 0$ and $y(0) = y_0$. This problem is a well-conditioned one. When the midpoint rule is applied to it, one obtains, by posing $q = h\lambda$,

$$y_{n+2} - 2qy_{n+1} - y_n = 0.$$

For every negative value of q, the characteristic polynomial of this equation has one root inside and one outside the unit disk. Consequently, it is not possible to control the parasitic root if both the two conditions required by the discrete problem are imposed at the initial points. In this form, the method cannot be used to solve the problem. This is no more the case, when one condition is imposed at the initial point and the other at the final one, as it can be easily checked. In this case, we say that the method has been used with $(1,1)$-*boundary conditions*.

In general, given the k-step formula for approximating (3),

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h \sum_{i=0}^{k} \beta_i f_{n+i}, \tag{5}$$

and two natural numbers k_1 and k_2, $k_1 + k_2 = k$, we say that the formula is used with (k_1, k_2)-*boundary conditions* if k_1 conditions, say $y_0, \ldots, y_{k_1-1}$, are given at the initial points, and k_2, say $y_N, \ldots, y_{N+k_2-1}$, are given at the final ones.

In recent years, such an idea has been exploited and the usual concepts of 0-stability, A-stability, and convergence have been generalized.

To get an overview of such results, we need to fix some essential notation and give some preliminary definitions. Let

$$\rho(z) = \sum_{i=0}^{k} \alpha_i z^i, \qquad \sigma(z) = \sum_{i=0}^{k} \beta_i z^i,$$

and for any complex q,

$$\pi(z, q) = \rho(z) - q\sigma(z)$$

be the usual polynomials characterizing the LMF (5).

DEFINITION 1. *A polynomial $p(z)$ of degree $k = k_1 + k_2$ is a $S_{k_1 k_2}$-polynomial if its roots are such that*

$$|z_1| \leq \cdots \leq |z_{k_1}| < 1 < |z_{k_1+1}| \leq \cdots \leq |z_k|.$$

DEFINITION 2. *A polynomial $p(z)$ of degree $k = k_1 + k_2$ is a $N_{k_1 k_2}$-polynomial if*

$$|z_1| \leq \cdots \leq |z_{k_1}| \leq 1 < |z_{k_1+1}| \leq \cdots \leq |z_k|$$

being simple the roots of unit modulus.

The above definitions generalize the usual notions of Schur and von Neumann polynomials, respectively. In fact, when $k_1 = k$ and $k_2 = 0$ (that is, when all the conditions for the discrete problem are given at the initial points), one easily verifies that a N_{k0}-polynomial reduces to a von Neumann polynomial, and a S_{k0}-polynomial is a Schur polynomial.

In order to stress the importance of such polynomials to our problem, we mention the following result which extends to discrete problems the discussion previously made for continuous ones.

THEOREM 1. *Let*

$$\sum_{i=0}^{k} p_i y_{n+i} = 0$$

be a linear difference equation with constant coefficients, whose characteristic polynomial has the roots satisfying the inequalities

$$|z_1| \leq \cdots \leq |z_{k_1-1}| < |z_{k_1}| < |z_{k_1+1}| \leq \cdots \leq |z_k|,$$
$$|z_{k_1-1}| < 1 < |z_{k_1+1}|.$$

Then, the discrete solution, obtained by imposing k_1 conditions at $n = 0, \ldots, k_1 - 1$ and k_2 conditions at $n = N, \ldots, N + k_2 - 1$, behaves, for n and $N - n$ large, as

$$y_n = z_{k_1}^n \left(\gamma + O\left(\left| \frac{z_{k_1}}{z_{k_1+1}} \right|^{N-n} \right) + O\left(|z_{k_1+1}|^{-N} \right) \right) + O\left(|z_{k_1-1}|^n \right) + O\left(|z_{k_1+1}|^{-(N-n)} \right), \tag{6}$$

where γ depends only on the initial conditions.

PROOF. (See [2,3].) Because of the form of the discrete solution (6), which is "essentially" given by $\gamma z_{k_1}^n$, z_{k_1} is called *generating root*.

In particular, when the difference equation is obtained by means of a suitable multistep method approximating a linear differential equation, such as, for example (4), and the used stepsize h is suitably small, then z_{k_1} will be an approximation to a certain order p of $e^{h\lambda}$,

$$z_{k_1} \equiv z_{k_1}(q) = e^q + O\left(h^{p+1}\right), \qquad q = h\lambda.$$

The usual stability notions are then generalized as follows.

DEFINITION 3. *A boundary value method used with (k_1, k_2)-boundary conditions is $0_{k_1 k_2}$-stable if the corresponding polynomial $\rho(z)$ is a $N_{k_1 k_2}$-polynomial.*

DEFINITION 4. *The region $\mathcal{D}_{k_1 k_2}$ of the complex plane defined by*

$$\mathcal{D}_{k_1 k_2} = \{q \in \mathbb{C} : \pi(z, q) \text{ is a } S_{k_1 k_2}\text{-polynomial}\}$$

is said region of (k_1, k_2)-absolute stability of the method.

From Theorem 1, it follows that the methods suitable to be used as BVMs are those for which

$$\inf_{q \in \mathcal{D}_{k_1 k_2}} |z_{k_1+1}(q)| > 1 \geq \sup_{q \in \mathcal{D}_{k_1 k_2}} |z_{k_1}(q)|.$$

DEFINITION 5. *A BVM used with (k_1, k_2)-boundary conditions is said to be $A_{k_1 k_2}$-stable if $\mathbb{C}^- \subseteq \mathcal{D}_{k_1 k_2}$.*

Observe that when $k_1 = k$ and $k_2 = 0$, the corresponding classical notions are obtained. The usual concept of convergence is then defined with minor changes. In particular, it can be shown that (in exact arithmetic) consistency and $0_{k_1 k_2}$-stability imply convergence [2,3].

Another set which has a relevance for a LMF is its *boundary locus*,

$$\Gamma = \left\{ q \in \mathbb{C} : q = \frac{\rho\left(e^{i\theta}\right)}{\sigma\left(e^{i\theta}\right)},\ 0 \leq \theta < 2\pi \right\}.$$

In fact, when Γ is a Jordan curve, then $\Gamma \equiv \partial \mathcal{D}_{k_1 k_2}$, the boundary of the (k_1, k_2)-absolute stability region of the method.

It is well known that the notion of absolute stability has its origin from the necessity to obtain asymptotically stable critical points for the discrete equations, when the continuous problems behave alike. Namely, such notion has been an effective tool to derive methods whose solutions

retain the qualitative behavior of the continuous ones around asymptotically stable equilibrium points. The fact that this is defined for the linear test equation (4) is not a severe limitation, as stated by the theorem of first approximation stability, which holds true for both continuous and discrete dynamical systems. Such theorem asserts that, under certain mild hypotheses, if a critical point is asymptotically stable for the linearized problem, the same will be true for the nonlinear one. This result is basic for Applied Mathematics. In fact, it permits us to linearize the problems around the critical solutions, and to study the linearized problems.

This important tool, however, is no more sufficient to study the behavior of systems which do not have asymptotically stable solutions. This is the case, for example, of Hamiltonian problems. Therefore, for such systems the analysis based on the test equation (4) is no longer sufficient. The additional request, in this case, is to have the discrete solution generated by a symplectic map (see, for example, [4–6]).

Let us give some more details on this point. For simplicity, the discussion will be restricted to the linear case. Given the linear Hamiltonian system

$$y' = Ly \equiv \begin{pmatrix} O_m & -I_m \\ I_m & O_m \end{pmatrix} Sy, \qquad S = S^T \in \mathbb{R}^{2m\times 2m}, \tag{7}$$

where I_m and O_m are the identity and the null $m \times m$ matrices, respectively, a one-step method of the form

$$y_{n+1} = R(hL)y_n,$$

should have $R(hL)$ symplectic, that is,

$$R(hL)^T \begin{pmatrix} O_m & -I_m \\ I_m & O_m \end{pmatrix} R(hL) = \begin{pmatrix} O_m & -I_m \\ I_m & O_m \end{pmatrix}.$$

This is the case of trapezoidal rule, for which

$$R(hL) = \left(I - \frac{1}{2}hL\right)^{-1}\left(I + \frac{1}{2}hL\right).$$

It turns out that this method is the only stable symplectic method in the class of LMF, when they are used as initial value methods (i.e., with only initial conditions).

In general, Theorem 1, which is stated for scalar difference equations, can be extended to the matrix difference equations derived from the application of method (5) to problem (7). The result is that the solution is essentially generated by a matrix, say $z_{k_1}(hL)$. Once again, "essentially" means that the other contributions are negligible. One has then

$$y_{n+1} \approx z_{k_1}(hL)y_n.$$

In this case, one requires the matrix $z_{k_1}(hL)$, which is called *generating matrix*, to be symplectic. Such methods have been called *"essentially" symplectic* [7].

Let us now review some classical families of LMF, along with their generalizations as BVMs, and compare their stability regions.

3. BDF AND GBDF

A family of LMF, extensively used in the solution of stiff ODE problems, is that of Backward Differentiation Formulae (BDF), defined by

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = hf_{n+k}. \tag{8}$$

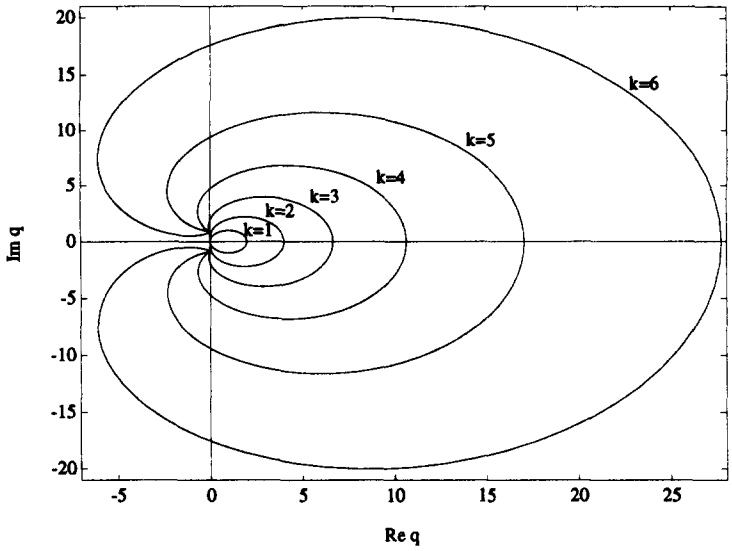

Figure 3. Boundary loci of BDF up to $k = 6$.

For each $k \geq 1$, the coefficients $\{\alpha_i\}$ are determined so that the formula has the maximum order k. However, such formulae provide stable methods only until $k = 6$. It is in fact known that the BDF of order 7 is 0-unstable (see, for example, [8]). The boundary loci of the stable BDF are reported in Figure 3, where the absolute stability regions are those outside the corresponding boundary loci.

The generalization of such methods as Boundary Value Methods amounts to evaluate the function f at an intermediate point, that is,

$$\sum_{i=0}^{k} \alpha_i y_{n+i} = h f_{n+\nu},$$

where ν is chosen as follows:

$$\nu = \begin{cases} \dfrac{k+2}{2}, & \text{for even } k, \\ \dfrac{k+1}{2}, & \text{for odd } k. \end{cases}$$

The resulting methods, called *Generalized BDF (GDBF)* [2,3], still have order k. For all $k \geq 1$, they must be used with $(\nu, k-\nu)$-boundary conditions and are $0_{\nu,k-\nu}$-stable. Their boundary loci are shown in Figure 4, for k odd, and in Figure 5, for k even, up to $k = 30$. The stability regions are the unbounded sets outside the corresponding boundary loci. From these pictures, one easily realizes that all these formulae are also $A_{\nu,k-\nu}$-stable. The improvement over the original methods is then evident.

In Table 1, the coefficients of the GBDF are reported for $k = 1, \ldots, 8$. For convenience, we report the normalized coefficients $\hat{\alpha}_i = \alpha_i \eta_k$, $i = 0, \ldots, k$.

4. ADAMS-MOULTON METHODS AND THEIR GENERALIZATION

The methods in this family are defined by the formula

$$y_{n+k} - y_{n+k-1} = h \sum_{i=0}^{k} \beta_i f_{n+i},$$

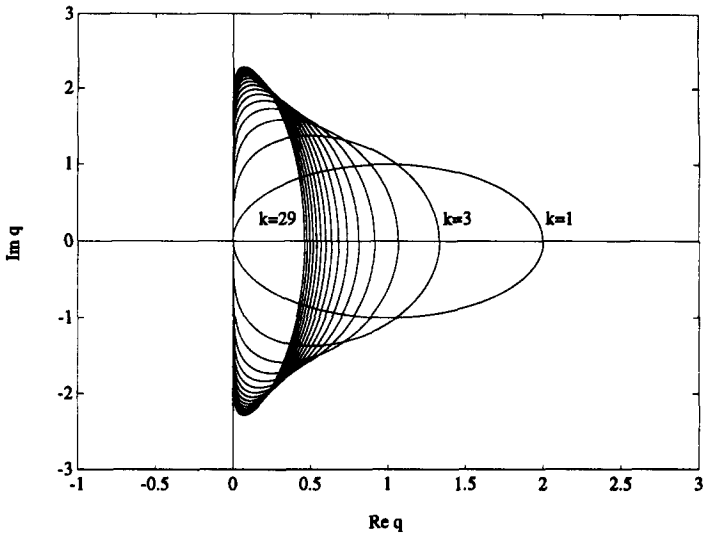

Figure 4. Boundary loci of GBDF, odd values of k.

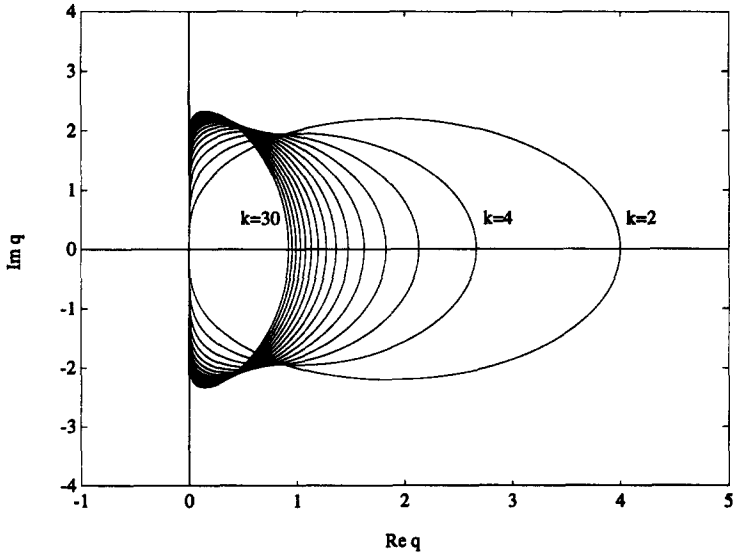

Figure 5. Boundary loci of GBDF, even values of k.

Table 1. Coefficients of GBDF.

k	ν	η_k	$\hat{\alpha}_0$	$\hat{\alpha}_1$	$\hat{\alpha}_2$	$\hat{\alpha}_3$	$\hat{\alpha}_4$	$\hat{\alpha}_5$	$\hat{\alpha}_6$	$\hat{\alpha}_7$	$\hat{\alpha}_8$
1	1	1	−1	1							
2	2	2	1	−4	3						
3	2	6	1	−6	3	2					
4	3	12	−1	6	−18	10	3				
5	3	60	−2	15	−60	20	30	−3			
6	4	60	1	−8	30	−80	35	24	−2		
7	4	420	3	−28	126	−420	105	252	−42	4	
8	5	840	−3	30	−140	420	−1050	378	420	−60	5

where the coefficients $\{\beta_i\}$ are determined so that the maximum order $k+1$ is reached. These methods are extensively used, mainly for approximating the solution of nonstiff ODEs. This is because the only Adams-Moulton method having an unbounded absolute stability region is the

trapezoidal rule, which corresponds to the case $k = 1$. However, for $k \geq 2$, the absolute stability regions of these methods are all bounded and become smaller and smaller as k increases. In Figures 6 and 7, the boundary loci of the Adams-Moulton methods are shown up to $k = 8$. The absolute stability regions are the subregions bounded by the section of the boundary locus plotted with solid line. It is evident from the pictures that such regions become more entangled and smaller as k increases.

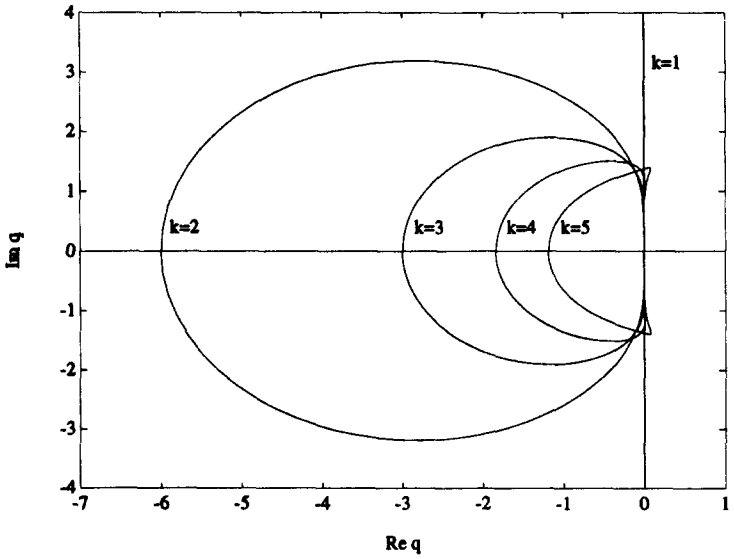

Figure 6. Boundary loci of the Adams-Moulton methods, $k = 1, \ldots, 5$.

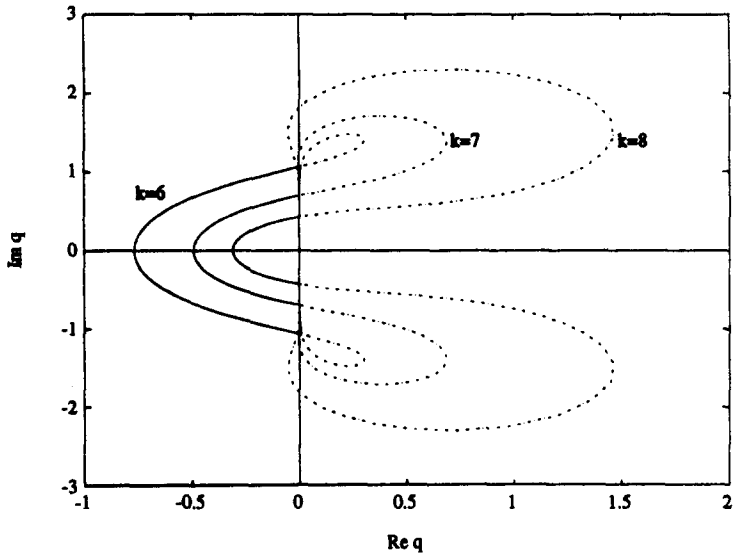

Figure 7. Boundary loci of the Adams-Moulton methods, $k = 6, 7, 8$.

The generalization of such methods as BVMs is described by the following formula:

$$y_{n+\nu} - y_{n+\nu-1} = h \sum_{i=0}^{k} \beta_i f_{n+i},$$

where ν is defined according to

$$\nu = \begin{cases} \dfrac{k+1}{2}, & \text{for odd } k, \\ \dfrac{k}{2}, & \text{for even } k. \end{cases}$$

The resulting methods, called *Generalized Adams Methods (GAMs)* [3], still have order $k+1$. For each $k \geq 1$, they must be used with $(\nu, k-\nu)$-boundary conditions, and are $0_{\nu,k-\nu}$-stable, $A_{\nu,k-\nu}$-stable methods.

In the next section, we shall consider the formulae with an odd number of steps. For the moment, we only report in Figure 8 the boundary loci of the methods with k even, up to $k = 30$. The corresponding stability regions are, obviously, the unbounded regions outside the corresponding boundary loci. Also in this case, the improvement over the original methods is evident.

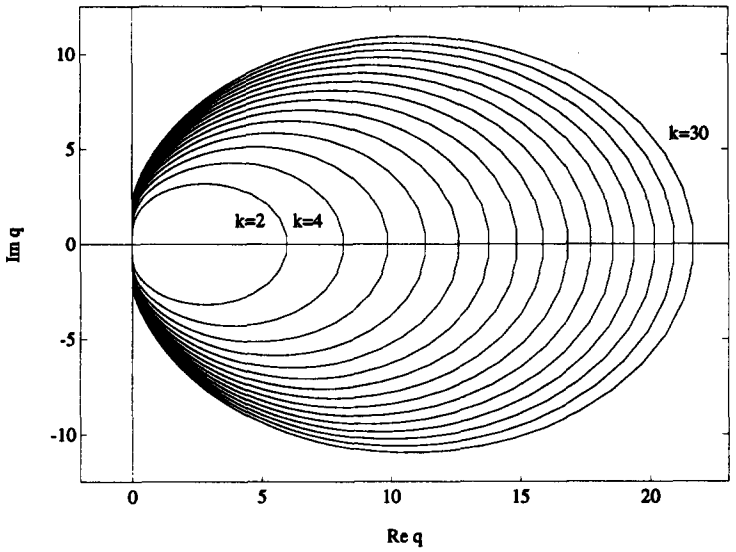

Figure 8. Boundary loci of GAMs, even values of k.

In Table 2, we report the coefficients of the GAMs for $k = 2, 4, 6$. Since the coefficients of $\rho(z)$ are fixed, only the coefficients of the polynomial $\sigma(z)$ are reported. For brevity, we report the normalized coefficients $\hat{\beta}_i = \beta_i \eta_k$, $i = 0, \ldots, k$.

Table 2. Coefficients of GAMs, k even.

k	ν	η_k	$\hat{\beta}_0$	$\hat{\beta}_1$	$\hat{\beta}_2$	$\hat{\beta}_3$	$\hat{\beta}_4$	$\hat{\beta}_5$	$\hat{\beta}_6$
2	1	12	−1	8	5				
4	2	720	11	−74	456	346	−19		
6	3	60480	−191	1608	−6771	37504	30819	−2760	271

5. SYMMETRIC SCHEMES

We group as *symmetric schemes* BVMs having the following general properties:

(1) an odd number of steps, $k = 2\nu - 1$, $\nu \geq 1$,

(2) the polynomials $\rho(z)$ with skew-symmetric coefficients,

$$\alpha_i = -\alpha_{k-i}, \qquad i = 0, \ldots, k, \tag{9}$$

(3) the polynomials $\sigma(z)$ with symmetric coefficients,

$$\beta_i = \beta_{k-i}, \qquad i = 0, \ldots, k. \tag{10}$$

LMF satisfying the above properties are unstable, when used with only initial conditions, for all $\nu > 1$. However, when used with $(\nu, \nu-1)$-boundary conditions, all the methods that we shall consider are $0_{\nu,\nu-1}$-stable and $A_{\nu,\nu-1}$-stable. Moreover, their boundary locus coincides with the imaginary axis, so that for all of them, one obtains

$$\mathcal{D}_{\nu,\nu-1} \equiv \mathbb{C}^-.$$

That is, the stability properties are exactly those of the trapezoidal rule,

$$y_n - y_{n-1} = \frac{h}{2}(f_n + f_{n-1}), \tag{11}$$

which is, in fact, the symmetric scheme corresponding to $\nu = 1$. This feature is very important because it states an equivalence between the stability regions of the continuous problem and of the discrete one.

Such methods are very important. In fact, they result to be the methods to be chosen when approximating either continuous boundary value problems [3,9] or Hamiltonian problems [3,10]. In particular, they are all "essentially" symplectic methods [7].

Three main families of symmetric schemes have been introduced. Each of them may be regarded as a suitable generalization of the basic trapezoidal rule (11).

ETRs. The *Extended Trapezoidal Rules* (ETRs) [3,11] are nothing but the GAMs with an odd number of steps. They have the following general form:

$$y_n - y_{n-1} = h\sum_{i=0}^{\nu-1} \beta_i (f_{n-\nu+i} + f_{n+\nu-1-i}), \tag{12}$$

where the coefficients $\{\beta_i\}$ are chosen so that the maximum order $k+1 = 2\nu$ is reached. In Table 3, we report the normalized coefficients $\hat{\beta}_i = \beta_i \eta_k$ of these methods, up to $k = 9$. Moreover, because of the symmetry (10), only the coefficients $\hat{\beta}_0, \ldots, \hat{\beta}_{\nu-1}$ are reported. For $\nu = 1$, one obtains the trapezoidal rule.

Table 3. Coefficients of ETRs.

k	ν	η_k	$\hat{\beta}_0$	$\hat{\beta}_1$	$\hat{\beta}_2$	$\hat{\beta}_3$	$\hat{\beta}_4$
1	1	2	1				
3	2	24	−1	13			
5	3	1440	11	−93	802		
7	4	120960	−191	1879	−9531	68323	
9	5	7257600	2497	−28939	162680	−641776	4134338

ETR_2s. ETRs can be regarded as generalizations of the trapezoidal rule preserving the structure of the first characteristic polynomial $\rho(z)$. Similarly, the *Extended Trapezoidal Rules of second kind* (ETR_2s) [3,7] can be considered as generalizations of (11) preserving the structure of the second characteristic polynomial $\sigma(z)$. Therefore, such methods will have the following form:

$$\sum_{i=0}^{\nu-1} \alpha_i (y_{n-\nu+i} - y_{n+\nu-1-i}) = \frac{h}{2}(f_n + f_{n-1}). \tag{13}$$

The coefficients $\{\alpha_i\}$ are determined so that the maximum possible order $p = k + 1$ is reached. In Table 4, we report the normalized coefficients $\hat{\alpha}_i = \alpha_i \eta_k$ of these methods, up to $k = 9$. Moreover, only the first ν coefficients are reported, since the remaining ones are obtained by the symmetry (9).

Table 4. Coefficients of ETR_2s.

k	ν	η_k	$\hat{\alpha}_0$	$\hat{\alpha}_1$	$\hat{\alpha}_2$	$\hat{\alpha}_3$	$\hat{\alpha}_4$
1	1	1	−1				
3	2	12	−1	−9			
5	3	120	1	−15	−80		
7	4	840	−1	14	−126	−525	
9	5	5040	1	−15	120	−840	−3024

Also in this case, for $\nu = 1$, one obtains the basic trapezoidal rule.

TOMs. The most general symmetric extension of the trapezoidal rule leads to methods in the form

$$\sum_{i=0}^{\nu-1} \alpha_i (y_{n-\nu+i} - y_{n+\nu-1-i}) = h \sum_{i=0}^{\nu-1} \beta_i (f_{n-\nu+i} + f_{n+\nu-1-i}). \tag{14}$$

In particular, for every $k = 2\nu - 1$, the maximum order $p = 2k$ for a k-step LMF can be reached. For this reason, such methods have been called *Top Order Methods* (TOMs) [3,12]. Their coefficients are given by [13]

$$\alpha_i = \frac{c_i - c_{k-i}}{c_k} \binom{k}{i}^2, \quad \beta_i = \frac{1}{2c_k} \binom{k}{i}^2, \qquad i = 0, \ldots, k,$$

where

$$c_0 = 0, \quad c_i = c_{i-1} + \frac{1}{i}, \qquad i \geq 1.$$

From these expressions, it is evident that the symmetries (9) and (10) are satisfied.

EXAMPLES. If the coefficients are normalized so that $\sum_i \beta_i = 1$, for $\nu = 1$, and then $k = 1$, the trapezoidal rule is again obtained. For $\nu = 2$, one obtains the sixth-order TOM,

$$\frac{1}{60}(11y_{n+1} + 27y_n - 27y_{n-1} - 11y_{n-2}) = \frac{h}{20}(f_{n+1} + 9f_n + 9f_{n-1} + f_{n-2}).$$

6. THE CHOICE OF THE ADDITIONAL CONDITIONS

We now consider the problem of providing the additional values needed by a BVM used with (k_1, k_2)-boundary conditions. Let us rewrite the chosen method as

$$\sum_{i=-k_1}^{k_2} \alpha_{i+k_1} y_{n+i} = h \sum_{i=-k_1}^{k_2} \beta_{i+k_1} f_{n+i}. \tag{15}$$

Here, we have assumed that the interval of integration $[t_0, T]$ has been partitioned according to

$$t_i = t_0 + ih, \qquad i = 0, \ldots, N + k_2 - 1, \qquad h = \frac{T - t_0}{N + k_2 - 1}.$$

Equation (15) can be used for $n = k_1, \ldots, N - 1$, thus, requiring the boundary conditions

$$y_0, y_1, \cdots, y_{k_1-1}, \qquad y_N, \cdots, y_{N+k_2-1}.$$

However, only the first of such values is available, since it is provided by the continuous problem. It is possible to treat the remaining $k - 1$ quantities as unknowns, by introducing a suitable set of $k - 1$ *additional equations* independent of those provided by the main formula (15). Such

equations can be conveniently derived by *additional methods* having the same order of (15). In particular, one usually considers $k_1 - 1$ additional *initial* equations,

$$\sum_{i=0}^{r} \alpha_i^{(j)} y_i = h \sum_{i=0}^{r} \beta_i^{(j)} f_i, \qquad j = 1, \ldots, k_1 - 1 \tag{16}$$

and k_2 *final* ones,

$$\sum_{i=0}^{r} \alpha_{r-i}^{(j)} y_{N+k_2-1-i} = h \sum_{i=0}^{r} \beta_{r-i}^{(j)} f_{N+k_2-1-i}, \qquad j = N, \ldots, N + k_2 - 1. \tag{17}$$

Here, for brevity, we have supposed all the additional methods having the same number of steps, that is r.

It can be shown that if the additional methods are appropriately chosen, the stability properties of the global method are inherited by the main formula (15) [3].

We observe that the discrete problem (15)–(17) only requires one more condition to be fixed, which is the one provided by the continuous problem. In this way, it is possible to extend the use of BVMs to the approximation of continuous boundary value problems, such as, for example,

$$y' = f(t, y), \qquad g(y(t_0), y(T)) = 0.$$

In fact, in this case, one simply completes the above set of equations with the boundary condition $g(y_0, y_{N+k_2-1}) = 0$ [3,9].

As an example, we mention the fourth-order ETR ($k_1 = 2$, $k_2 = 1$),

$$y_n - y_{n-1} = \frac{h}{24}(-f_{n+1} + 13f_n + 13f_{n-1} - f_{n-2}), \qquad n = 2, \ldots, N - 1,$$

which can be completed with the following two equations:

$$y_1 - y_0 = \frac{h}{24}(f_3 - 5f_2 + 19f_1 + 9f_0),$$
$$y_N - y_{N-1} = \frac{h}{24}(f_{N-3} - 5f_{N-2} + 19f_{N-1} + 9f_N),$$

both obtained by additional fourth-order methods. For each BVM previously considered, there exists an appropriate choice of the additional methods [3].

7. BLOCK VERSION

The arguments exposed in the last section allows us to consider a BVM and its corresponding additional methods, as a composite method. Having fixed a suitable N, such method allows us to pass from the approximation at $t = t_0$ to the one at $t = t_{N+k_2-1}$. For brevity, let us pose $s = N + k_2 - 1$. Then, one may think to discretize the interval $[t_0, T]$ by using two different meshes. Let the coarser mesh contain the $p + 1$ points

$$\tau_i = \tau_{i-1} + \hat{h}_i, \qquad i = 1, \ldots, p, \qquad \tau_0 \equiv t_0, \qquad \tau_p \equiv T.$$

Then, on each subinterval $[\tau_{i-1}, \tau_i]$, $i = 1, \ldots, p$, we apply the same (composite) BVM, as above described, by using the finer stepsize $h_i = \hat{h}_i / s$.

In more detail, by using the initial condition y_0 provided by the continuous problem (3), we can apply the BVM over the first subinterval $[\tau_0, \tau_1]$, with finer stepsize $h_1 = \hat{h}_1 / s$. The discrete approximation $\{y_{j1}\}$ of the solution at the points

$$t_j = \tau_0 + jh_1, \qquad j = 1, \ldots, s$$

is then obtained. In the used notation, the rightmost lower index of y_{j1} identifies the first subinterval.

One then uses the value $y_{s1} \approx y(\tau_1)$ for computing the approximated solution over the second subinterval $[\tau_1, \tau_2]$ with the same BVM. In this case, however, the used finer stepsize will be $h_2 = \hat{h}_2/s$.

It is evident that the process can be iterated $p-2$ more times, thus, providing a discrete approximation over the entire interval $[t_0, T]$.

The resulting procedure defines the *block version of BVMs*. The points used inside each block will be referred as *internal steps*. There is a resemblance between these methods and Runge-Kutta schemes, whose stages play a role similar to that of the internal steps. However, we observe that there is a substantial difference between the two classes of methods. In fact, the accuracy at the internal stages of a Runge-Kutta scheme is usually much worse than that at the final point. Conversely, for BVMs the accuracy at the internal steps, and at the final one, is exactly the same, provided that the additional methods are appropriately chosen.

The above defined block version of BVMs has two important practical implications, which make BVMs computationally effective.

The first one is that the stepsize variation becomes very simple: inside each block the used stepsize is constant, while one may vary the stepsize in the coarser mesh. This permits an easy use of mesh selection strategies [3,14].

The second relevant consequence is that the block version of BVMs allows also a very efficient parallel implementation of the methods [3,15].

8. NUMERICAL RESULTS

In this section, we report some numerical tests obtained by using a block version of BVMs. For brevity, we shall consider only two initial value problems, but several numerical tests, especially concerning the approximation of continuous BVPs, can be found elsewhere [3,14].

The first problem is a severe stiff test problem [16]

$$y' = A_\nu(t)y + f(t), \qquad t \in [0, 10\pi], \qquad y(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{18}$$

where

$$f(t) = \begin{pmatrix} -\sin(t) \\ \cos(t) \end{pmatrix} - A_\nu(t) \begin{pmatrix} \cos(t) \\ \sin(t) \end{pmatrix},$$

ν is a nonnegative parameter, and

$$A_\nu(t) = M_\nu(t) \begin{pmatrix} -1001 & 0 \\ 0 & -1 \end{pmatrix} M_\nu^T(t),$$
$$M_\nu(t) = \begin{pmatrix} \cos(\nu t) & \sin(\nu t) \\ -\sin(\nu t) & \cos(\nu t) \end{pmatrix}.$$

The solution of the problem is given by $y(t) = (\cos(t)\sin(t))^T$, independently of the value of the parameter ν. Despite the fact that the solution is very smooth, the problem is stiff. In fact, the eigenvalues of the matrix $A_\nu(t)$ are $\lambda_1 = -1$ and $\lambda_2 = -1001$, for all ν and t. Moreover, the problem becomes more and more difficult as the parameter ν is increased [17].

Since the solution of the problem is very smooth, it is reasonable to expect that high-order methods will perform well. For this reason, we consider the GBDF of order 20 with initial stepsize 0.1 on problem (18) with $\nu = 1000$. The stepsize is changed by using a tolerance 10^{-5} for the local errors. The integration interval is covered with 141 mesh points, and stepsizes ranging from 0.1 to 0.48. The maximum absolute error on the computed solution has been $\approx 2.5 \times 10^{-8}$.

The second problem is an Hamiltonian one,

$$y' = \begin{pmatrix} & -I_5 \\ I_5 & \end{pmatrix} Sy, \qquad y_0 = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \tag{19}$$

where I_r denotes the identity matrix of size r, $S = 8I_{10} + Q$, and the $(i,j)^{\text{th}}$ entry of Q is $i + j$, $i, j = 1, \ldots, 10$.

In this case, a parallel implementation with constant stepsize has been used. We have considered the ETRs with $k = 3, 5, 7, 9$ steps, implemented with $s = 20$ internal steps. The parallel algorithm has been executed on a transputer based machine, which is a distributed memory parallel computer. In Table 5, the execution times on one processor, and the measured speed-ups on p processors, are reported. The execution times are expressed in *ticks*, each corresponding to $64\,\mu$sec.

Table 5. Measured speed-ups for problem (19).

$p \setminus k$	3	5	7	9
1	1.00	1.00	1.00	1.00
2	1.95	1.99	1.99	1.99
4	3.77	3.91	3.94	3.96
8	7.34	7.67	7.77	7.85
16	14.16	15.05	15.34	15.55
time	63255	92055	127230	163485

By the way, we mention that, for linear Hamiltonian problems, the continuous invariants of the problem are exactly preserved at the extreme points of each block [3,10].

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